

Chapter 15 - THE SANS INSTRUMENTAL RESOLUTION

Instrumental smearing affects SANS data. In order to analyze smeared SANS data, either de-smearing of the data or smearing of the fitting model function is required. The second approach is more common because it is a direct method. Smearing corrections use the instrumental resolution function.

1. THE RESOLUTION FUNCTION

Instrumental smearing is represented by the following 1D convolution smearing integral (suitable for radially averaged data):

$$\left[\frac{d\Sigma(Q)}{d\Omega} \right]_{\text{smeared}} = \int_0^{+\infty} dQ' P_{1D}(Q') \frac{d\Sigma(Q-Q')}{d\Omega}. \quad (1)$$

Here Q is the scattering variable, $d\Sigma(Q)/d\Omega$ is the scattering cross section and the 1D resolution function is defined as a Gaussian function:

$$P_{1D}(Q') = \left(\frac{1}{2\pi\sigma_{Q'}^2} \right)^{1/2} \exp \left[-\frac{Q'^2}{2\sigma_{Q'}^2} \right]. \quad (2)$$

The Q standard deviation σ_Q is a measure of the neutron beam spot size on the detector ($Q = 0$). It is also a measure of the instrumental part of the width of scattering peaks from samples ($Q \neq 0$). σ_Q is related to the spatial standard deviation (i.e., standard deviation of the neutron beam spot at the detector) σ_r by $\sigma_Q = (2\pi/\lambda L_2)\sigma_r$, where L_2 is the sample-to-detector distance.

2. VARIANCE OF THE Q RESOLUTION

Scattering measurements are made in reciprocal (Fourier transform) space where the magnitude of the scattering vector is given by:

$$Q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right). \quad (3)$$

Here λ is the neutron wavelength and θ is the scattering angle. At small angles, Q is approximated by: $Q = 2\pi\theta/\lambda$.

In order to express σ_Q , differentiate Q on both sides:

$$dQ = \frac{2\pi}{\lambda} d\theta - \frac{2\pi}{\lambda^2} \theta d\lambda. \quad (4)$$

Take the square:

$$(dQ)^2 = \left(\frac{2\pi}{\lambda}\right)^2 (d\theta)^2 + \left(\frac{2\pi}{\lambda^2}\right)^2 \theta^2 (d\lambda)^2 - 2 \frac{(2\pi)^2}{\lambda^3} \theta (d\theta)(d\lambda). \quad (5)$$

Then perform the statistical averages:

$$\langle (dQ)^2 \rangle = \left(\frac{2\pi}{\lambda}\right)^2 \langle (d\theta)^2 \rangle + \frac{(2\pi)^2}{\lambda^4} \theta^2 \langle (d\lambda)^2 \rangle - 2 \frac{(2\pi)^2}{\lambda^3} \langle \theta (d\theta)(d\lambda) \rangle \quad (6)$$

Note that $\langle \theta (d\theta)(d\lambda) \rangle = \langle \theta (d\theta) \rangle \langle (d\lambda) \rangle$ because the scattering angle θ and the wavelength λ distributions are uncorrelated. Moreover,

$\langle (d\lambda) \rangle = \langle (\lambda - \langle \lambda \rangle) \rangle = \langle \lambda \rangle - \langle \lambda \rangle = 0$. This cancels out the last term.

Define the different **variances**:

$$\begin{aligned} \sigma_Q^2 &= \langle (dQ)^2 \rangle = \langle Q^2 \rangle - \langle Q \rangle^2, \\ \sigma_\theta^2 &= \langle (d\theta)^2 \rangle = \langle \theta^2 \rangle - \langle \theta \rangle^2, \\ \sigma_\lambda^2 &= \langle (d\lambda)^2 \rangle = \langle \lambda^2 \rangle - \langle \lambda \rangle^2 \end{aligned} \quad (7)$$

The SANS **resolution variance** has two contributions:

$$\sigma_Q^2 = [\sigma_Q^2]_{\text{geo}} + [\sigma_Q^2]_{\text{wav}} = \frac{4\pi^2}{\lambda^2} \sigma_\theta^2 + Q^2 \frac{\sigma_\lambda^2}{\lambda^2} \quad (8)$$

These correspond to the “**geometry**” part (first term) and to the “**wavelength spread**” part (second term) of the Q resolution variance.

3. SANS RESOLUTION VARIANCE

The main parts of the resolution variance σ_Q^2 are derived for a SANS instrument with circular apertures (Mildner-Carpenter, 1984; Mildner et al, 2005).

Geometry Contribution to the Q Resolution

Consider the geometry contribution to the Q resolution variance:

$$\sigma_0^2 = \frac{\sigma_r^2}{L_2^2} \quad (9)$$

L_2 is the sample-to-detector distance. The variance for the radially averaged data corresponds to 1D. The 1D case of σ_x^2 (in the horizontal x direction) is considered first.

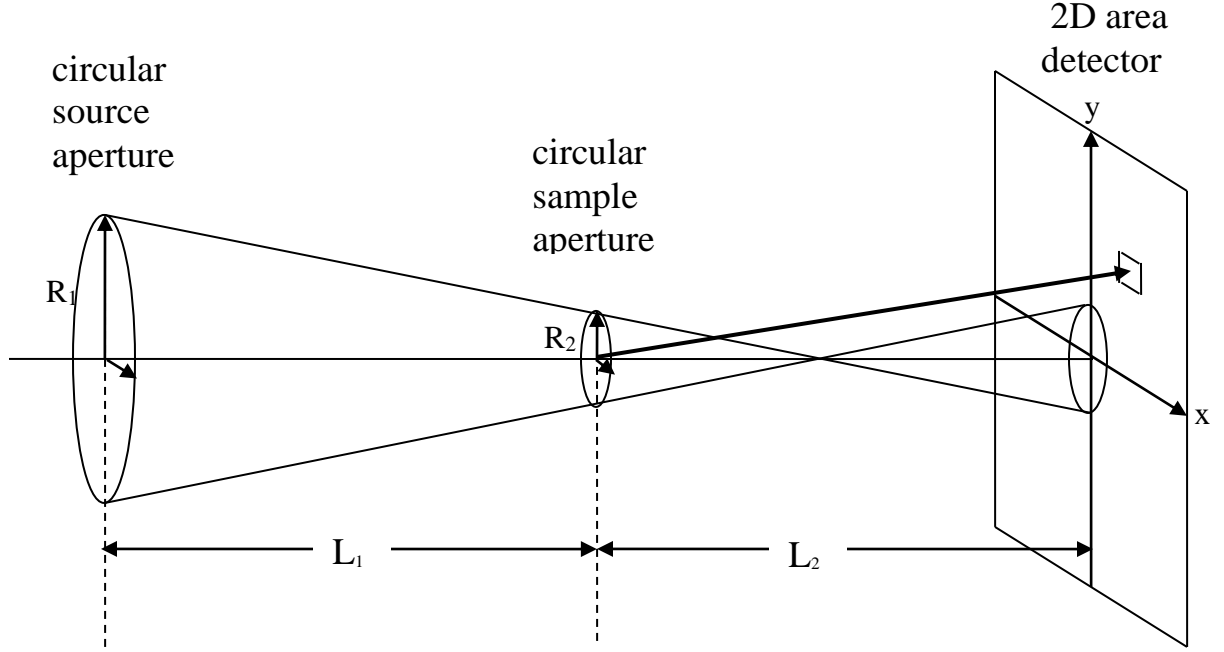


Figure 1: Typical SANS geometry with circular source and sample apertures and 2D area detector. This figure is not to scale. The horizontal scale is in meters whereas the vertical scale is in centimeters. Aperture sizes have been drawn out of scale compared to the size of the area detector.

Consider a uniform neutron distribution within the source and sample apertures. The horizontal contribution can be written:

$$\sigma_x^2 = \left(\frac{L_2}{L_1}\right)^2 \langle x^2 \rangle_1 + \left(\frac{L_1 + L_2}{L_1}\right)^2 \langle x^2 \rangle_2 + \langle x^2 \rangle_3. \quad (10)$$

L_1 is the source-to-sample distance, L_2 is the sample-to-detector distance, $\langle x^2 \rangle_1$ is the averaging over the source aperture, $\langle x^2 \rangle_2$ is the averaging over the sample aperture and $\langle x^2 \rangle_3$ is the averaging over a detector cell. R_1 and R_2 define the source and sample aperture radii respectively. In order to see the origin of the (L_2/L_1) scaling factor, consider the case where $R_2 = 0$. Then the spot at the detector would be similar to the source aperture size scaled by (L_2/L_1) . Similarly, in order to see the origin of the $(L_1 + L_2)/L_1$

scaling factor, consider the case of $R_1 = 0$. The spot would be similar to the sample aperture size scaled by $(L_1 + L_2)/L_1$.

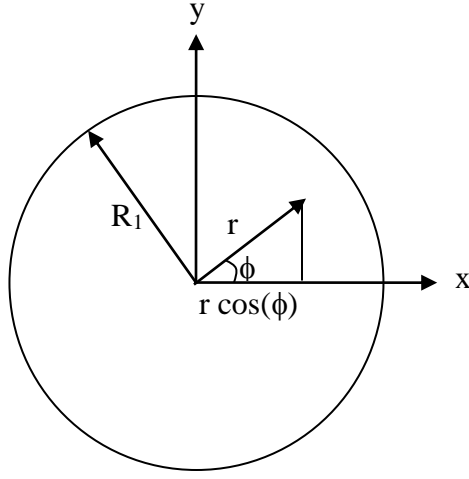


Figure 2: Geometry of the circular source aperture.

The various averages can be readily calculated:

$$\langle x^2 \rangle_1 = \frac{\int_0^{2\pi} \int_0^{R_1} r^2 \cos^2(\phi) r dr d\phi}{\int_0^{2\pi} \int_0^{R_1} r dr d\phi} = \frac{\int_0^{R_1} r^3 dr \int_0^{2\pi} \cos^2(\phi) d\phi}{\int_0^{R_1} r dr \int_0^{2\pi} d\phi} = \frac{R_1^2}{4}. \quad (11)$$

Similarly $\langle x^2 \rangle_2 = \frac{R_2^2}{4}$. Averaging over the square (or rectangular) detector cell of sides Δx_3 and Δy_3 follows.

$$\langle x^2 \rangle_3 = \frac{\int_{-\Delta x_3/2}^{\Delta x_3/2} dx x^2}{\int_{-\Delta x_3/2}^{\Delta x_3/2} dx} = \frac{\Delta x_3^2}{12} = \frac{1}{3} \left(\frac{\Delta x_3}{2} \right)^2. \quad (12)$$

Therefore:

$$\sigma_x^2 = \left(\frac{L_2}{L_1} \right)^2 \frac{R_1^2}{4} + \left(\frac{L_1 + L_2}{L_1} \right)^2 \frac{R_2^2}{4} + \frac{\Delta x_3^2}{12}. \quad (13)$$

Similarly for the vertical part (assuming no effect of gravity on the neutron trajectory):

$$\sigma_y^2 = \left(\frac{L_2}{L_1}\right)^2 \frac{R_1^2}{4} + \left(\frac{L_1 + L_2}{L_1}\right)^2 \frac{R_2^2}{4} + \frac{\Delta y_3^2}{12}. \quad (14)$$

So that:

$$\begin{aligned} \left[\sigma_{Qx}^2\right]_{\text{geo}} &= \left(\frac{2\pi}{\lambda}\right)^2 \frac{\sigma_x^2}{L_2^2} \\ \left[\sigma_{Qy}^2\right]_{\text{geo}} &= \left(\frac{2\pi}{\lambda}\right)^2 \frac{\sigma_y^2}{L_2^2} \end{aligned} \quad (15)$$

This is the first part of the Q resolution variance.

Wavelength Spread Contribution to the Q Resolution

The neutron wavelength is assumed to obey a triangular distribution peaked around λ and of full-width at half maximum $\Delta\lambda$.

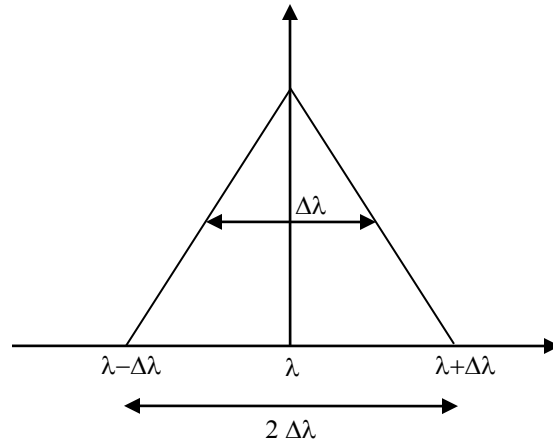


Figure 3: **Triangular wavelength distribution.**

This is a typical distribution outputted by a velocity selector. For simplicity of notation, the same symbol λ is used to denote both the wavelength variable λ and the average wavelength $\langle\lambda\rangle$. The average over this wavelength distribution can be readily calculated as:

$$\langle \lambda^2 \rangle = \lambda^2 \left[1 + \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \right]. \quad (16)$$

Note that if we had assumed a square (also called “box”) wavelength distribution, the factor of 1/6 would be replaced by 1/12.

The wavelength variance is therefore:

$$\frac{\sigma_{\lambda}^2}{\lambda^2} = \frac{(\langle \lambda^2 \rangle - \langle \lambda \rangle^2)}{\lambda^2} = \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2. \quad (17)$$

The wavelength spread contribution to the Q resolution variance is therefore as follows:

$$\begin{aligned} [\sigma_{Q_x}^2]_{\text{wav}} &= Q_x^2 \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \\ [\sigma_{Q_y}^2]_{\text{wav}} &= Q_y^2 \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \end{aligned} \quad (18)$$

This is the second part of the Q resolution variance.

Neutron Trajectories

Gravity affects neutron trajectories. Consider neutrons of wavelength λ and wavelength spread $\Delta \lambda$ incident on the source aperture. The initial neutron velocity is v_0 with components v_{0y} and v_{0z} along the vertical and horizontal directions.

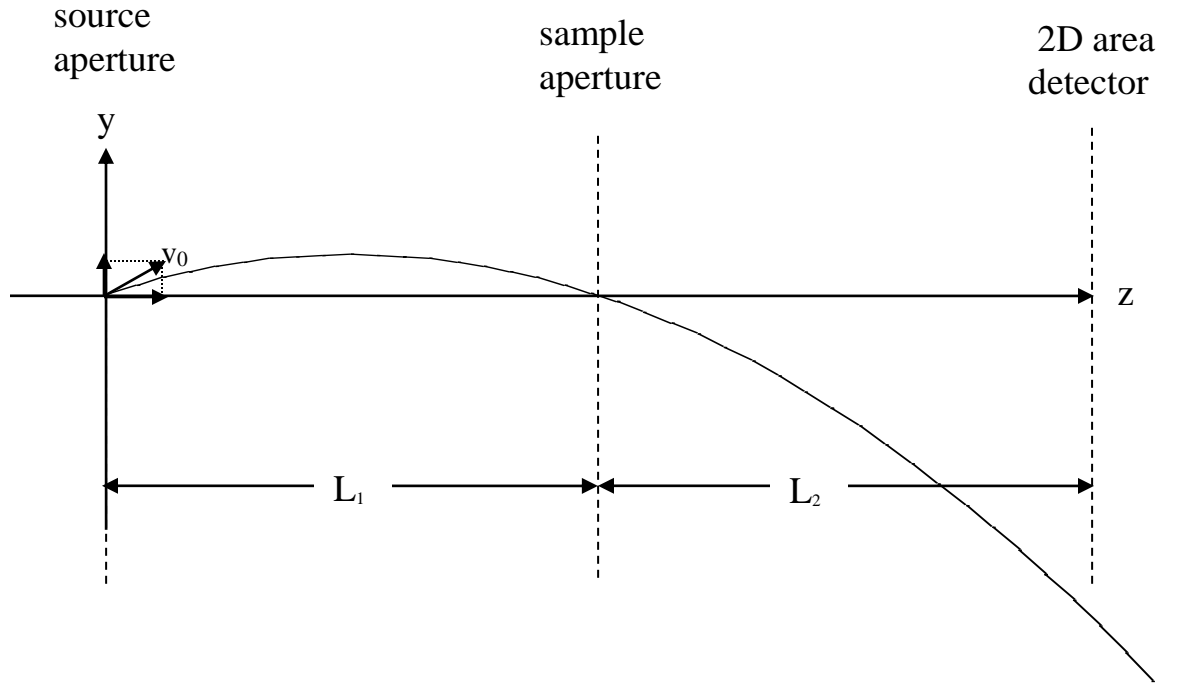


Figure 4: **Parabolic neutron trajectory under gravity effect**. Neutrons must cross the source and sample apertures. This figure is not to scale.

Under the effect of gravity, neutrons follow the following trajectories:

$$z = v_{0z} t \quad (19)$$

$$y = y_0 - \frac{1}{2} g t^2 + v_{0y} t.$$

Here g is the gravity constant ($g = 9.81 \text{ m/s}^2$) and t is time. Neutrons are assumed to be at the horizontal axis origin at time zero. In order to obtain the neutron trajectories equation, the time variable is eliminated using the fact that neutrons must cross the source and sample apertures; i.e., the condition $y = y_0$ for $z = 0$ and for $z = L_1$. This gives:

$$\begin{aligned} L_1 = v_{0z} t & \Rightarrow t = \frac{L_1}{v_{0z}} \\ y_0 = -\frac{1}{2} g t^2 + v_{0y} t & \Rightarrow v_{0y} = y_0 + \frac{1}{2} g \frac{L_1}{v_{0z}}. \end{aligned} \quad (20)$$

The horizontal neutron speed v_{0z} is related to the neutron wavelength λ by:

$$v_{0z} = \frac{h}{m\lambda}. \quad (21)$$

Here also, h is Planck's constant and m is the neutron mass. At any other position along the neutron path (other than $z = 0$ and $z = L_1$), the parabolic variation followed is:

$$y(z) = y_0 - \frac{1}{2}g\left(\frac{m\lambda}{h}\right)^2 (z^2 - zL_1) = y_0 - B\lambda^2(z^2 - zL_1) \quad (22)$$

where:

$$B = \frac{gm^2}{2h^2}. \quad (23)$$

The neutron fall trajectory is characterized by a parabolic variation with respect to z and with respect to λ .

For $z = L_1 + L_2$, neutrons fall by the distance $y(L_1 + L_2) = y_0 - B\lambda^2 L_2(L_1 + L_2)$.

Effect of Gravity on the Q Resolution

Gravity affects the fall of the neutron and therefore the resolution in the y direction. Neutron trajectories follow a parabola:

$$y = y_0 - A\lambda^2 \quad \text{with} \quad A = BL_2(L_1 + L_2) \quad \text{and} \quad B = \frac{gm^2}{2h^2}. \quad (24)$$

g is the gravitation constant ($g = 9.81 \text{ m/s}^2$), m is the neutron mass and h is Plank's constant ($h/m = 3995 \text{ \AA.m/s}$). $A = 3.073 \cdot 10^{-7} L_2(L_1 + L_2)$ given in units of m/\AA^2 where L_1 and L_2 are the source-to-sample and sample-to-detector distances given in meters.

The gravity contribution to the Q_y variance is given by:

$$\left[\sigma_{Q_y}^2\right]_{\text{grav}} = \left(\frac{2\pi}{\lambda}\right)^2 \frac{\left[\sigma_y^2\right]_{\text{grav}}}{L_2^2} \quad (25)$$

$$\left[\sigma_y^2\right]_{\text{grav}} = \langle (y - y_0)^2 \rangle - \langle (y - y_0) \rangle^2 = A^2 (\langle \lambda^4 \rangle - \langle \lambda^2 \rangle^2).$$

The two averages over the triangular wavelength distribution are performed as follows:

$$\begin{aligned} \langle \lambda^2 \rangle &= \lambda^2 \left[1 + \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \right] \\ \langle \lambda^4 \rangle &= \lambda^4 \left[1 + \left(\frac{\Delta \lambda}{\lambda} \right)^2 + \frac{1}{15} \left(\frac{\Delta \lambda}{\lambda} \right)^4 \right]. \end{aligned} \quad (26)$$

Therefore:

$$\langle \lambda^4 \rangle - \langle \lambda^2 \rangle^2 \cong \lambda^4 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda} \right)^2. \quad (27)$$

So that:

$$\left[\sigma_y^2 \right]_{\text{grav}} = A^2 \lambda^4 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda} \right)^2. \quad (28)$$

and finally:

$$\left[\sigma_{Q_y}^2 \right]_{\text{grav}} = \left(\frac{2\pi}{L_2} \right)^2 A^2 \lambda^2 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda} \right)^2. \quad (29)$$

This term is added in quadrature with the other two contributions (geometry and wavelength spread) to the Q resolution variance σ_Q^2 .

Summary of the Q Resolution

Putting the geometry contribution, the wavelength spread contribution and the gravity contribution together yields:

$$\sigma_{Q_x}^2 = \left(\frac{2\pi}{\lambda L_2} \right)^2 \left[\left(\frac{L_2}{L_1} \right)^2 \frac{R_1^2}{4} + \left(\frac{L_1 + L_2}{L_1} \right)^2 \frac{R_2^2}{4} + \frac{1}{3} \left(\frac{\Delta x_3}{2} \right)^2 \right] + Q_x^2 \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \quad (30)$$

$$\sigma_{Q_y}^2 = \left(\frac{2\pi}{\lambda L_2} \right)^2 \left[\left(\frac{L_2}{L_1} \right)^2 \frac{R_1^2}{4} + \left(\frac{L_1 + L_2}{L_1} \right)^2 \frac{R_2^2}{4} + \frac{1}{3} \left(\frac{\Delta y_3}{2} \right)^2 + A^2 \lambda^4 \frac{2}{3} \left(\frac{\Delta \lambda}{\lambda} \right)^2 \right] + Q_y^2 \frac{1}{6} \left(\frac{\Delta \lambda}{\lambda} \right)^2$$

$$A = L_2 (L_1 + L_2) \frac{g m^2}{2 h^2}$$

where:

R_1 : source aperture radius
 R_2 : sample aperture radius
 Δx_3 and Δy_3 : sides of the detector cell
 L_1 : source-to-sample distance
 L_2 : sample-to-detector distance
 $\Delta\lambda$: wavelength spread, FWHM of triangular distribution function
 g : gravity constant
 m : neutron mass
 h : Planck's constant.

This result was obtained assuming a uniform neutron distribution within the apertures and a triangular wavelength distribution.

4. MINIMUM Q

A figure of merit for SANS instruments is the minimum value of the scattering variable Q (also called Q_{\min}) that can be reached for a given configuration. This value is imposed by the neutron spot size on the area detector and dictates the size of the beamstop to be used. In order to minimize the spot size, one has to minimize the “umbra” and “penumbra” of the neutron beam.

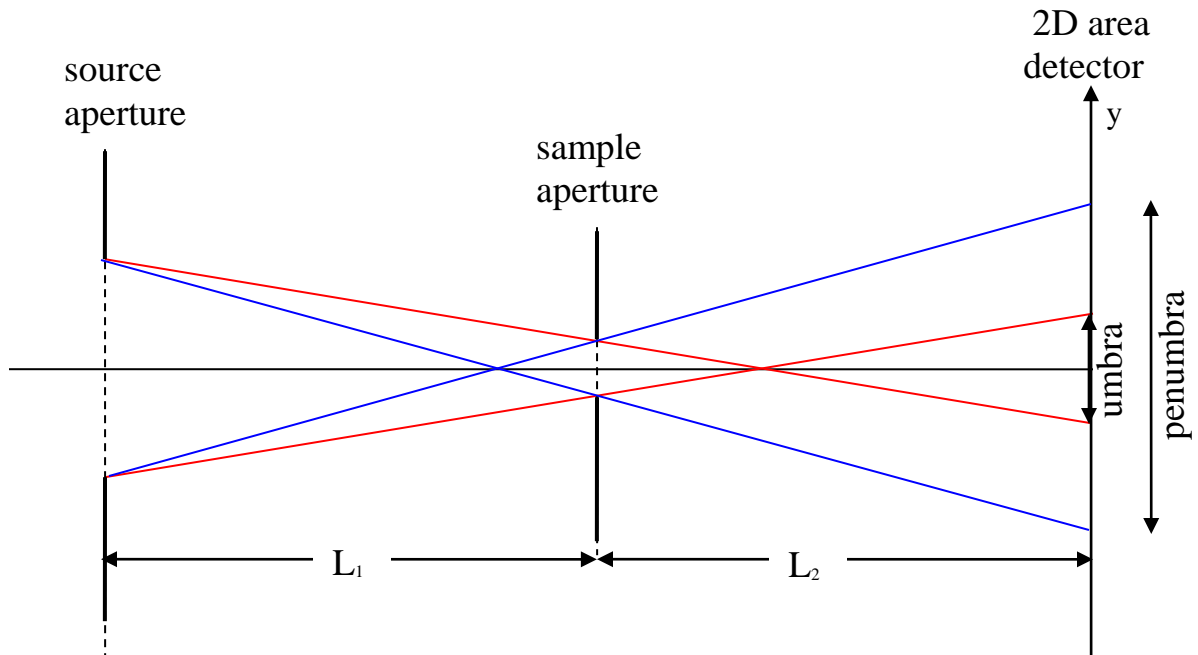


Figure 5: Converging collimation geometry to minimize spot size. This figure is not to scale. The penumbra is the maximum spot size to be blocked by the beamstop.

Given the standard SANS geometry, the extent of the penumbra in the horizontal direction is given by:

$$X_{\min} = \frac{L_2}{L_1} R_1 + \frac{L_1 + L_2}{L_1} R_2 + \frac{\Delta x_3}{2}. \quad (31)$$

And the minimum Q in the horizontal direction is therefore $Q_{\min}^X = (2\pi/\lambda)(X_{\min}/L_2)$.

In the vertical direction, the effect of gravity plays a role. The upper edge of the penumbra moves down by $A(\lambda - \Delta\lambda)^2$ because it corresponds to faster neutrons with wavelength $\lambda - \Delta\lambda$. The lower edge of the penumbra drops down by more; i.e., by $A(\lambda + \Delta\lambda)^2$ because it corresponds to slower neutrons with wavelength $\lambda + \Delta\lambda$. This results in a distorted beam spot at the detector. To first order in wavelength spread, one obtains:

$$Y_{\min} = \frac{L_2}{L_1} R_1 + \frac{L_1 + L_2}{L_1} R_2 + \frac{\Delta y_3}{2} + 2A\lambda^2 \left(\frac{\Delta\lambda}{\lambda} \right). \quad (32)$$

Note that Q_{\min} is determined by the spot size in the vertical direction where the beam is the broadest $Q_{\min} = Q_{\min}^Y = (2\pi/\lambda)(Y_{\min}/L_2)$.

$$Q_{\min} = \left(\frac{2\pi}{\lambda L_2} \right) \left(\frac{L_2}{L_1} R_1 + \frac{L_1 + L_2}{L_1} R_2 + \frac{\Delta y_3}{2} + 2A\lambda^2 \left(\frac{\Delta\lambda}{\lambda} \right) \right). \quad (33)$$

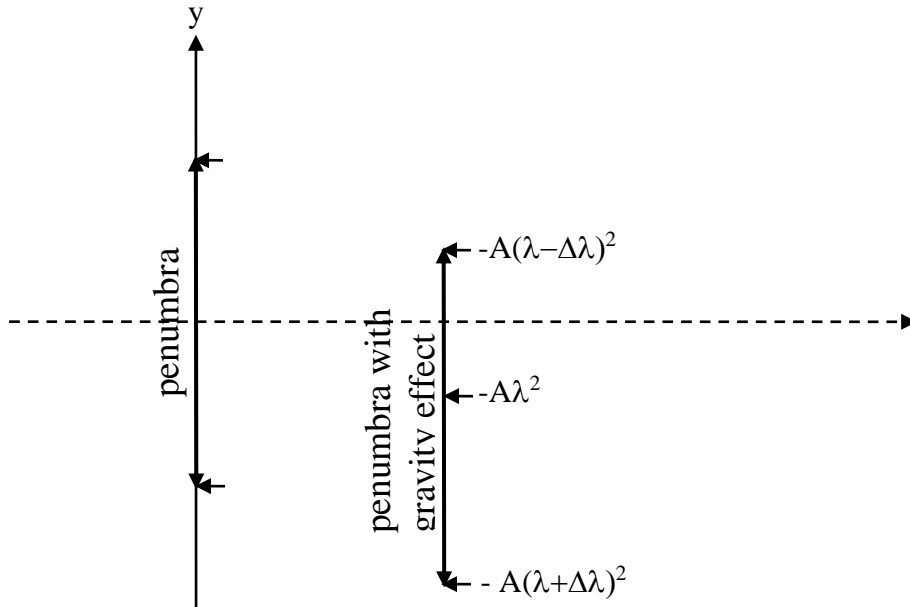


Figure 6: Neutron spot on the detector. The effect of gravity is to drop both the upper edge and the lower edge of the penumbra. The lower edge drops more resulting in distorted iso-intensity contours.

5. MEASURED SANS RESOLUTION

Specific Instrument Configuration

Consider the following low-Q instrument configuration.

$$\begin{aligned}L_1 &= 16.14 \text{ m} \\L_2 &= 13.19 \text{ m} \\R_1 &= 0.715 \text{ cm} \\R_2 &= 0.635 \text{ cm} \\\Delta x_3 = \Delta y_3 &= 0.5 \text{ cm} \\\frac{\Delta \lambda}{\lambda} &= 0.13.\end{aligned}$$

This gives a gravity fall parameter of $A = 0.01189 \text{ cm}/\text{\AA}^2$. This configuration does not strictly obey the “cone rule” whereby the beam spot umbra at the detector is minimized.

Assuming a neutron wavelength of $\lambda = 6 \text{ \AA}$, the variance σ_Q^2 has the following Q dependence:

$$\sigma_Q^2 = 2.76 * 10^{-7} + 0.0028 Q^2 (\text{\AA}^{-2}). \quad (34)$$

The minimum scattering variable is:

$$Q_{\min} = 0.0017 \text{\AA}^{-1}. \quad (35)$$

Gravity effects are small for 6 \AA neutrons. Neutrons fall by only 0.428 cm .

The focus here will be on empty beam measurement (i.e., with no sample in the beam). This corresponds to the resolution limit of $Q = 0$.

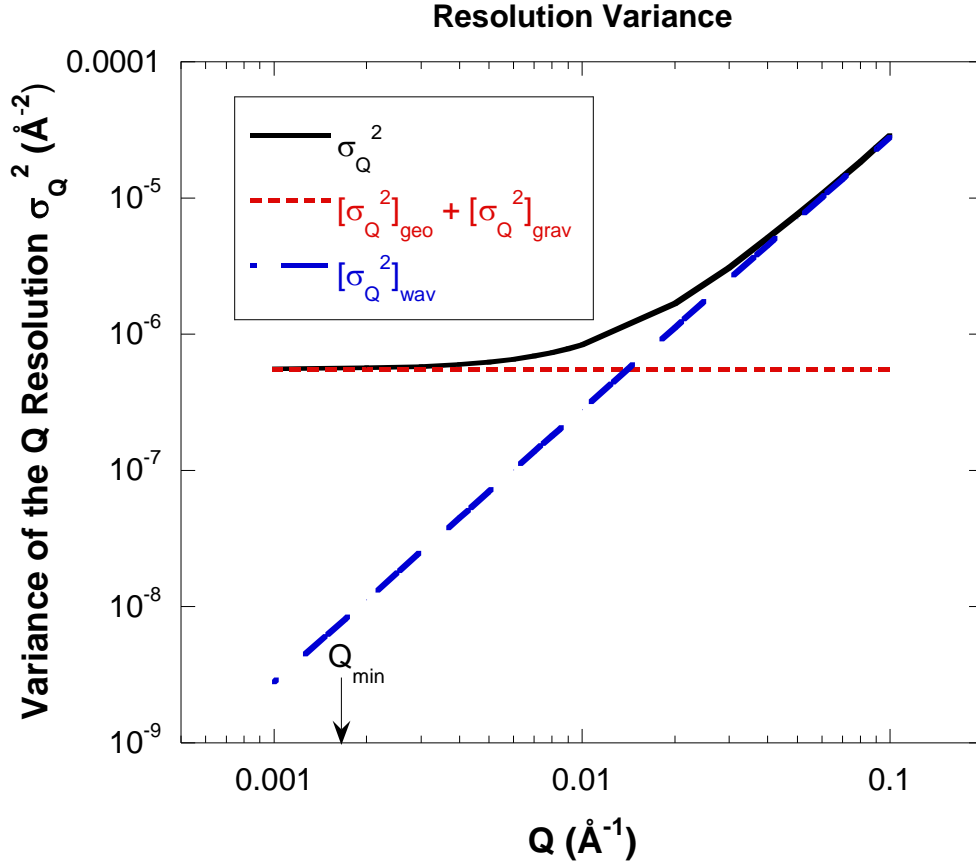


Figure 7: Variation of σ_Q^2 with Q plotted on a log-log scale. The main contributions (geometry, wavelength spread and gravity effect) are added in quadrature.

Empty Beam Measurements

Empty beam measurements were made using the above instrument configuration and varying the neutron wavelength.

Predicted and measured resolution characteristics are compared in a series of figures. First, the position of the beam spot on the detector is plotted for increasing wavelength.

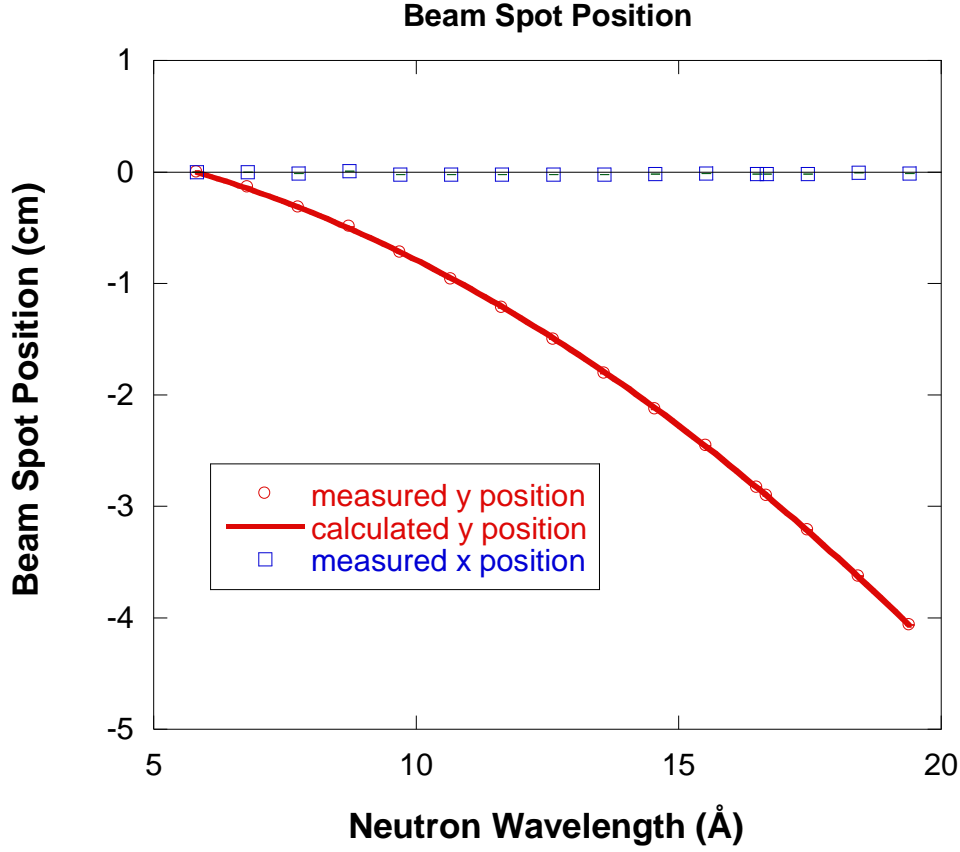


Figure 8: Variation of the horizontal and vertical neutron beam spot positions with wavelength.

Next, the standard deviations σ_x and σ_y of the neutron spot size are plotted with increasing neutron wavelength. The measured values were obtained by performing non-linear least-squares fits to a Gaussian function in the x and in the y directions. Fits were performed on cuts through the beam spot center, both horizontally and vertically. Data recorded by two adjacent detector cells (normal to the cut) were added in each case in order to improve statistics. A scaling factor of $\sqrt{1.45} = 1.2$ was used to scale the measured data. This scaling factor gave good agreement between the measured and calculated values for σ_x . The same scaling factor was used for σ_y .

This necessary scaling factor of 1.2 is probably related to the procedure used to obtain measured beam spot widths. (1) Slice cuts were performed in the horizontal and vertical directions. (2) Gaussian fits were performed on these slices even though the beam profile is known to be close to a trapezoidal (not Gaussian) shape. (3) Lastly, the measured beam spots were so small (covering only a few detector cells) that Gaussian fits were performed with four to eight points only.

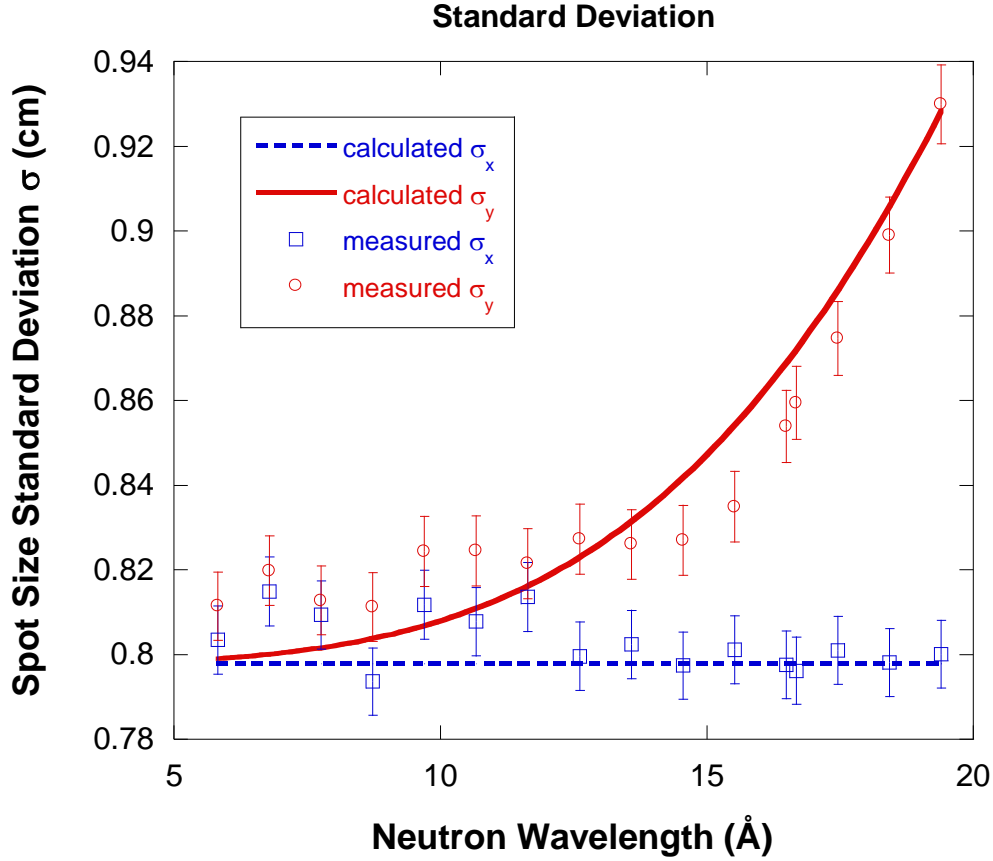


Figure 9: Variation of the measured and calculated neutron beam spot size standard deviations σ_x and σ_y with increasing wavelength.

The minimum spot sizes X_{\min} and Y_{\min} were obtained experimentally as the values where the intensity (of the horizontal or vertical cuts across the beam spot) goes to zero. This method is conservative and overestimates the measured values for X_{\min} . It is not precise, yielding poor agreement between measured and calculated values. Our calculated values neglect for instance diffuse scattering from the beam defining sample aperture and from the pre-sample and post-sample neutron windows. Such scattering tends to broaden the neutron beam. At long wavelengths, the gravity effect broadens the neutron spot in the vertical direction with the extra difference $Y_{\min} - X_{\min}$ given by the term $2\lambda^2(\Delta\lambda/\lambda)$.

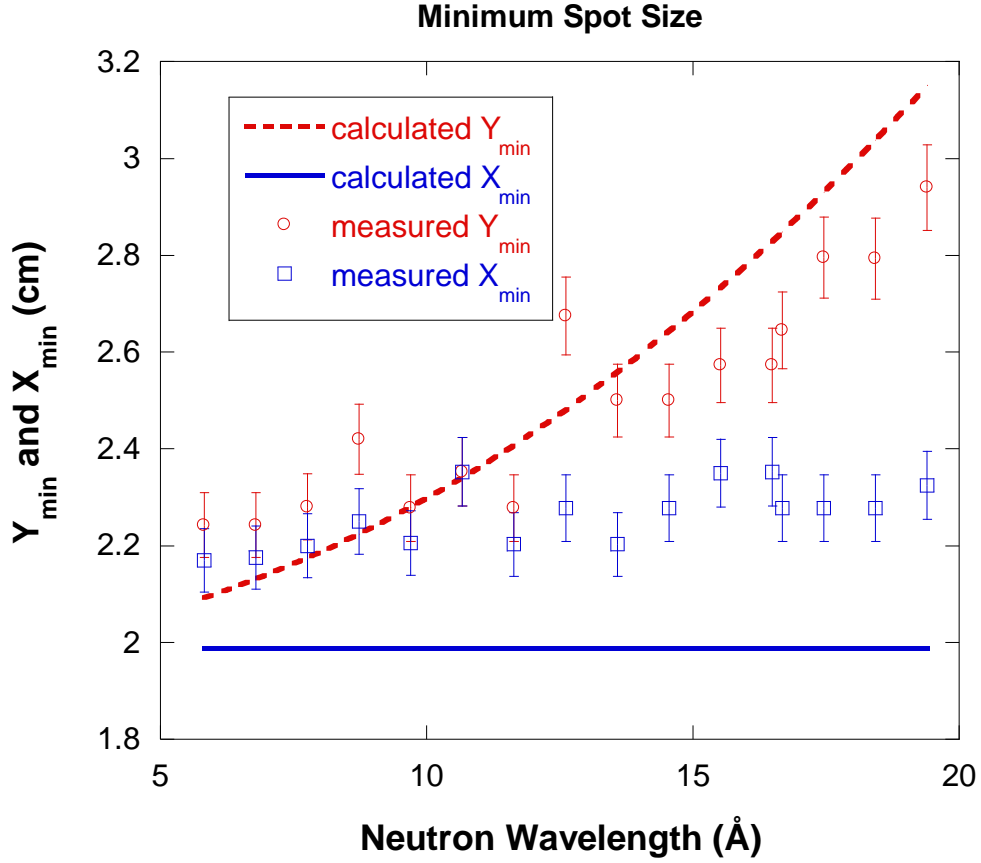


Figure 10: Variation of the neutron beam spot sizes in the horizontal and vertical directions with increasing wavelength.

6. DISCUSSION

The choice of a SANS instrument configuration is always a compromise between high intensity and good resolution. The instrumental resolution is the main source of data smearing. Estimation of the SANS resolution is an integral part of the data reduction process. Reduced SANS data include not only the scattering variable Q and the scattered intensity $I(Q)$, but also the resolution standard deviation σ_Q . σ_Q is needed to smear models before fitting to the data.

Corrections for smearing due to gravity are never made because they are small and deemed to be complex manipulations of the 2D data. The effect of gravity smearing is small except at long neutron wavelengths. Fortunately, the wide majority of experiments maximize flux by using low wavelengths (5 Å or 6 Å).

REFERENCES

D.F.R. Mildner, J.M. Carpenter, "Optimization of the Experimental Resolution for SAS", J. Appl. Cryst. 17, 249-256 (1984).

D.F.R. Mildner, B. Hammouda, and S.R. Kline, "A Refractive Focusing Lens System for SANS", J. Appl. Cryst. 38, 979-987 (2005).

QUESTIONS

1. What is the relationship between the standard deviation and the variance of a peaked function?
2. What function best describes the wavelength distribution function after the velocity selector?
3. What is the shape of the penumbra of the neutron beam spot on the detector?
4. Given a Gaussian function, what is the relationship between its FWHM and its standard deviation σ ?
5. Calculate the following average $\langle \lambda^2 \rangle$ over a triangular wavelength distribution. Calculate $\langle \lambda^2 \rangle$ over a Gaussian wavelength distribution of standard deviation σ_λ .
6. What are the various contributions to the SANS instrumental resolution?
7. The gravity effect is worse at what wavelength range?
8. What is the shape of the neutron beam spot on the detector for long wavelengths?
9. Cold neutrons of 20 Å wavelength fall by how much over a distance of 30 m?
10. Name the main "figures of merit" for a SANS instrument.
11. How would you obtain a lower Q_{\min} ?
12. If it takes 4 seconds for a pebble to reach the water level of a well, how deep is the well?

ANSWERS

1. The variance σ_Q^2 is the square of the standard deviation σ_Q .
2. The wavelength distribution after the velocity selector is best described by a triangular function.
3. The neutron beam spot on the detector has a shape close to trapezoidal.
4. For a Gaussian distribution, the following relationship holds $\text{FWHM} = 2\sqrt{2\ln(2)} \sigma$. In order to derive this relation, consider a Gaussian function $P(x) = (1/2\pi\sigma^2)^{1/2} \exp(-x^2/2\sigma^2)$ with standard deviation σ . Setting $P(x) = 1/2$, two solutions can be found for $x = \pm \sqrt{2\ln(2)} \sigma$. This yields a band $\text{FWHM} = 2\sqrt{2\ln(2)} \sigma = 2.355\sigma$.
5. The integrations are simple. Only the results are given.

$$\langle \lambda^2 \rangle = \lambda^2 \left[1 + \frac{1}{6} \left(\frac{\Delta\lambda}{\lambda} \right)^2 \right] \text{ for triangular distribution of FWHM } \Delta\lambda.$$

$$\langle \lambda^2 \rangle = \lambda^2 \left[1 + \left(\frac{\sigma_\lambda}{\lambda} \right)^2 \right] \text{ for Gaussian distribution of standard deviation } \sigma_\lambda.$$

6. The SANS instrumental resolution contains contributions from (1) “geometry” (source, sample aperture and detector cell sizes and source, sample and detector inter-distances), (2) from “wavelength spread” and (3) from “gravity” effect. Remember that $[\sigma_Q^2]_{\text{geo}} \sim \text{constant}$, $[\sigma_Q^2]_{\text{wav}} \sim Q^2(\Delta\lambda/\lambda)^2$ and $[\sigma_Q^2]_{\text{grav}} \sim \lambda^4(\Delta\lambda/\lambda)^2$.
7. The effect of gravity is worse for longer wavelengths.
8. Neutrons fall more at the bottom of the neutron beam than at the top. For this reason, beam spot iso-intensity contour maps are weakly elliptical (weakly oval actually).
9. Cold neutrons of 20 Å wavelength fall by about 4 cm over a distance of 30 m (see Figure 8).
10. Typical figures of merit for SANS instrument include: resolution σ_Q , Q_{min} , flux-on-sample, Q -range (called ΔQ) and background level.
11. A lower Q_{min} could be obtained by increasing the sample-to-detector distance. When this distance is at its maximum, then one could increase the neutron wavelength. The reason for this is that the beam intensity (1) decreases as sample-to-detector distance square but (2) it decreases as neutron wavelength to the fourth power.
12. The pebble falls according to the law of gravity $y = gt^2 / 2$ where $g = 9.81 \text{ m/s}^2$ is the gravity constant and t is time. After a time $t = 4 \text{ s}$, the pebble would have fallen $y = 9.81 * 4^2 / 2 \approx 78.5 \text{ m}$.